Mixed-Mode Calculations in Nuclear Physics

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Abstract

The one-dimensional harmonic oscillator in a box problem is used to introduce the concept of a mixed-mode shell-model scheme. The method combines low-lying "pure mode" states of a system to achieve a better description in situations where complete calculations cannot be done and the dynamics is driven by a combination of modes. The scheme is tested for real nuclei by combining traditional spherical states, which yield a diagonal representation of the single-particle interaction, with collective SU(3) configurations that track deformation. An application to the ds-shell ^{24}Mg nucleus, using the realistic two-body interaction of Wildenthal, is explored to test the validity of the concept. The results shown that the mixed-mode scheme reproduces the correct binding energy of ^{24}Mg (within 2% of the exact result) as well as low-energy configurations that have greater than 90% overlap with exact solutions in a space that spans less than 10% of the full space. In the pf-shell, the Kuo-Brown-3 interaction is used to illustrate coherent structures of the low-lying states of ^{48}Cr. Alternative basis sets are suggested for future mixed-mode shell-model studies.

Typically, two competing modes characterize the structure of a nuclear system. One is the single-particle mode that is the underpinning of the mean-field concept; the other is the many-particle collective behavior manifested in the nuclear deformation. The spherical shell model is the theory of choice when single-particle behavior dominates [1]. When deformation dominates, the Elliott SU(3) model can be used successfully [2]. This manifests itself in two dominant elements in the nuclear Hamiltonian: the single-particle term $H_0 = \sum_i \varepsilon_i n_i$ and a collective quadrupole-quadrupole interaction $H_{QQ} = Q \cdot Q$. It follows that a simplified Hamiltonian $H = \sum_i \varepsilon_i n_i - \chi Q \cdot Q$ has two solvable limits.

To probe the nature of such a system, we first consider a simpler problem: the one-dimensional harmonic oscillator in a box of size $2L$ [3]. As is the case for real nuclei, this system has a finite volume and a harmonic restoring potential, $\omega^2 x^2/2$. Depending on the value of $E_c = \omega^2 L^2/2$, which plays the role of a critical energy, there are three spectral types:

(1) For $\omega \to 0$ the energy spectrum is simply that of a particle in a box.

(2) At some value of ω, the energy spectrum begins with E_c followed by the spectrum of a particle in a box perturbed by the harmonic oscillator potential.

(3) For sufficiently large ω there is a harmonic oscillator spectrum below E_c and a perturbed spectrum of a particle in a box above E_c.

The last scenario (3) is the most interesting one, since it provides an example of a two-mode system. For this case, the use of two sets of basis vectors, one representing each of the two limits, has physical appeal for energies around E_c. One basis set consists of the harmonic oscillator states; the other set consists of basis states of a particle in a box. We call this combination a mixed-mode / oblique-basis approach. In general, the oblique-basis vectors form a nonorthogonal and sometimes an overcomplete set. Even though a mixed spectrum is expected around E_c, our numerical study which included up to 50 harmonic oscillator states below E_c, shows that first-order, energy-based perturbation theory works well after a breakdown in the harmonic oscillator spectrum.

Although the spectrum seems to be well described using first order perturbation theory, the wave functions near E_c have an interesting coherent structure. For example, the zero order approximation to the wave function used to calculate the energy may not be present in the structure of the exact wave function. Another feature is the common shape of the distribution that is similar to the coherent mixing observed in nuclei [4].

An application of the theory to the ds-shell nucleus ^{24}Mg [5], using the realistic two-body interaction of Wildenthal [6], demonstrates the validity of the mixed-mode shell-model scheme. In this case the oblique-basis consists of the traditional spherical states, which yield a diagonal representation of the single-particle interaction, together with collective SU(3) configurations, which yield a diagonal quadrupole-quadrupole interaction. The results obtained in a space that spans less than 10% of the full-space reproduce the correct binding energy (within 2% of the full-space result), as well as the low-energy spectrum and structure of the states that have greater than 90% overlap with the full-space results. In contrast, for a m-scheme spherical shell-model calculation one needs about 60% of the full space to obtain comparable results.

Studies of the lower pf-shell nuclei $^{44-48}Ti$ and ^{48}Cr [4] using the realistic Kuo-Brown-3 (KB3) interaction [7] show that the SU(3) symmetry breaking is due mainly to the single-particle spin-orbit splitting. Thus the KB3 Hamiltonian could also be considered a two-mode system. This has been further supported by the behavior of the yrast band B(E2) values that seems to be insensitive to fragmentation of the SU(3) symmetry. Specifically, the quadrupole collectivity as measured by the B(E2) strengths remains high even though the SU(3) symmetry is rather badly broken. This has been attributed to a quasi-SU(3) symmetry [8] where the observables behave like a pure SU(3) symmetry while the true eigenvectors exhibit a strong coherent structure with respect to each of the two bases. This provides an opportunity for further study of the implications of two-mode calculations.

Future research may extend this to multi-mode calculations. An immediate extension of the current scheme might use the eigenvectors of the pairing interaction [9] within the Sp(4) algebraic approach to nuclear structure [10], with the collective SU(3) states and spherical shell model states. Hamiltonian driven basis sets can also be considered. In particular, the method may use eigenstates of the very-near closed shell nuclei obtained from a full shell model calculation to form Hamiltonian driven J-pair states for mid-shell nuclei [11]. This type of extension would mimic the Interacting Boson Model (IBM) [12] and the so-called broken-pair theory. In particular, the three exact limits of the IBM [13] can be considered to comprise a three-mode system. Nonetheless, the real benefit of this approach is expected when the system is far away of any exactly solvable limit of the Hamiltonian and the spaces encountered are too large to allow for exact calculations.

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